

# sulfadimethoxine

**Inchi:** InChI=1S/C12H14N4O4S/c1-19-11-7-10(14-12(15-11)20-2)16-21(17,18)9-5-3-8(13)4-6-9  
**InchiKey:** ZZORFUFYDOWNEF-UHFFFAOYSA-N  
**Formula:** C12H14N4O4S  
**SMILES:** COc1cc(NS(=O)(=O)c2ccc(N)cc2)nc(OC)n1  
**Mol. weight [g/mol]:** 310.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Aqueous Solubility Prediction Method
logp	0.877		Crippen Method
mcvol	212.170	ml/mol	McGowan Method
tf	476.98	K	Aqueous Solubility Prediction Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**tf:** Normal melting (fusion) point

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